ANNUAL PROGRESS REPORT YEAR 2- 2001

Project Title:	Modeling and Optimization of Direct Chill Casting to Reduce Ingot Cracking
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Recipient:	Secat, Inc., 1505 Bull Lea Road Coldstream Research Campus Lexington, KY 40511
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Other Partners:	Alcan Aluminum Corp. ARCO Aluminum, Inc. Commonwealth Aluminum Logan Aluminum McCook Metals, LLC Wagstaff, Inc
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Project Objective:

The objective of the project is to develop a detailed model of thermal conditions, solidification, micro structural evolution, stress development, and cracking during the initial transient in DC casting. In particular, the program will
Conduct experimental measurements of extremely non-uniform heat removal at the ingot surface under industrial environments,
Characterize the ingot distortion and microstructure in detail,
Develop computer models of DC casting process for predicting the fluid flow, temperature, and stress fields, and micro structural evolution,
Determine material properties and develop a criterion for crack formation based on a fundamental understanding of the interaction between the solidification microstructure, the local stress, and solidification conditions,
Demonstrate and validate the models for predicting crack formation, and optimizing process parameters and ingot geometry, for a commercial installation,

Implement the models developed in this project in a commercial code so that they will be accessible to industry and be amenable to refinement in the future.

By
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Status

A team comprising of Secat industrial members, university personnel, and national laboratory researchers has been formed. In order to achieve the objectives of the project, four research groups were formed. Table 1 lists the members of the four research groups. Each group will focus on specific tasks as follows:

- Group 1 will conduct experimental measurements of heat removal and the ingot surface under industrial environments,
- Group 2 will characterize the solidification microstructure and the ingot distortion in detail,
- Group 3 will develop computer models of the DC casting process for predicting the fluid flow, temperature, and stress fields, and microstructural evolution,
- Group 4 will determine the material properties and develop a criterion for crack formation based on a fundamental understanding of the interaction between the solidification microstructure, the local stress, and solidification conditions.

Table 1. Research Groups in DC Casting Cracking Reduction Program

Group 1 Heat Transfer Measurements	Group 2 Ingot Dimensions and Microstructure	Group 3 Macro-Models Heat, Fluid, and Stress	Group 4 Micro-Models Cracking Criterion
Davis (Wagstaff) Saito (UK) - Kuwana - Hassan Clark (ARC) Sabau (ORNL) - Viswanathan	Davis (Wagstaff) Clark (ARC) Han (ORNL) - Viswanathan	Saito (UK) - Kuwana - Hassan, Li Sabau (ORNL) - Viswanathan	Saito, Hassan (UK) Krumdick (ANL) - Almer, Haeffner - Hryn Han (ORNL) - Ice - Viswanathan

In Year 2, significant progress was made and notable achievements were realized. A 2D model of the DC casting process has been developed in order to calculate HTCs at the ingot surface using an inverse method and the experimental data measured at the Wagstaff trial. An electrolytic etching technique was developed to reveal the grain size of the ingot. The microstructure in a transverse section near the location of the surface cracking was characterized. Microstructural length scales, such as grain size and secondary dendrite arm spacing, have been measured. Thermodynamic simulations were carried out to determine the solidus temperature, the solid fraction curve and the segregation behavior of the alloy during solidification.

Kinetic simulations were carried out to determine the solidus temperature of the alloy as a function of cooling rate. An experimental apparatus for measuring the mechanical properties of alloys in the critical temperature range for surface cracking has been assembled. The apparatus is being calibrated and property measurements are ongoing.

1. Heat Transfer Measurements

Objective:

- Calculate heat transfer coefficients (HTCs) at the ingot surface using an inverse technique using thermocouple data obtained at Wagstaff, Inc.

Year 2 Activities:

- Developed a 2D model of the DC casting process.
- Compared calculated temperatures with measured thermocouple data in order to validate model and obtain a reasonable first guess of HTCs.
- Performed inverse calculations to with first guess of HTCs and experimentally obtained thermocouple data to obtain heat transfer coefficients at the ingot surface.
- Compared temperatures obtained by the inverse calculation with measured thermocouple data to confirm that the model is reasonable.

Results/Summary:

A 2D model of the DC casting process has been developed in order to calculate HTCs at the ingot surface using an inverse method and the experimental data measured at the Wagstaff trial. The model was developed in ProCAST, a commercial software package for the simulation of casting processes. The model includes fluid flow and solidification. Four heat transfer regimes are considered in the model: 1) water cooling region that includes convection, nucleate boiling and film boiling, 2) air gap region, 3) mold/ingot interface region, and 4) starting block/ingot interface region. Casting parameters such as casting speed and pouring temperature are taken into account in the model. Thermo physical properties of the alloy were based on our measurements and a literature survey.

Since the inverse calculation is computationally expensive, it is important to make the initial assumption of HTCs as reasonable as possible. We took the initial values of HTCs from previous studies on DC casting available in the literature. Temperatures computed from the first values of HTCs were compared with experimentally obtained thermocouple data. Computed temperatures agreed reasonably with measurements.

Figures 1 and 2 show typical distributions of solid fraction and temperature. It can be seen that the ingot surface temperature becomes significantly lower (less than 150°C) after nucleate boiling starts. In addition, the mushy zone becomes thinner and temperature gradient becomes bigger after nucleate boiling starts.

The temperature history obtained by the inverse calculation is plotted in Figure 3. Measured temperature and temperature calculated from the initial guess of HTCs are also plotted in the same figure. Temperature obtained by the inverse calculation has better agreement with the experimentally measured temperature, although there is still significant variation between the measured and calculated values. Further refinements to the model are ongoing.

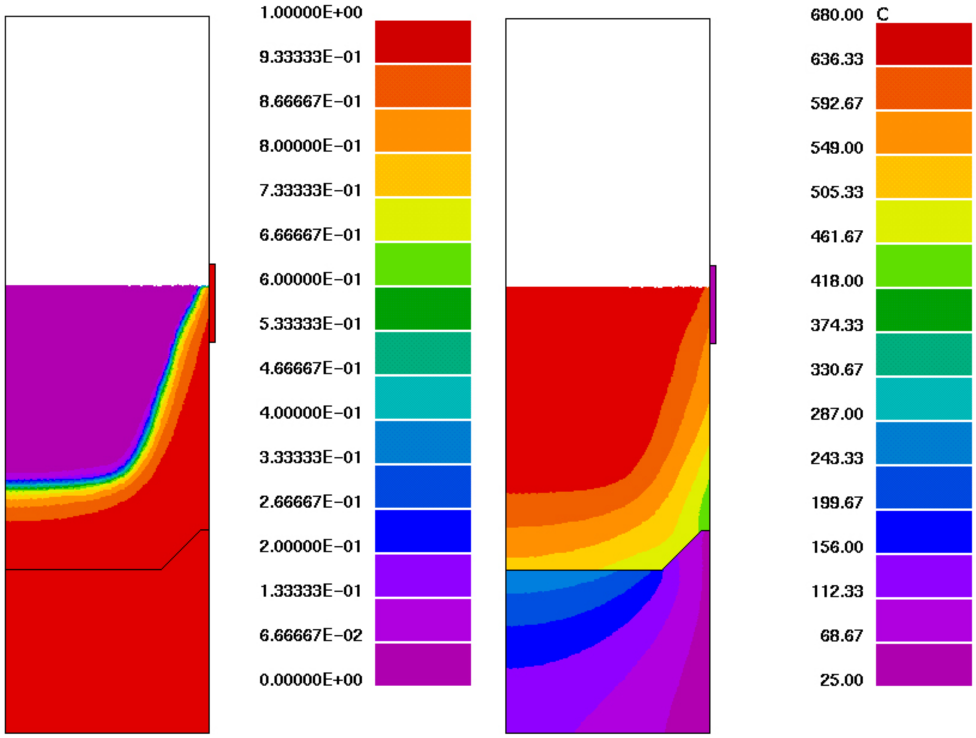

Fig 1: Solid fraction (left) and temperature (right) before nucleate boiling starts.

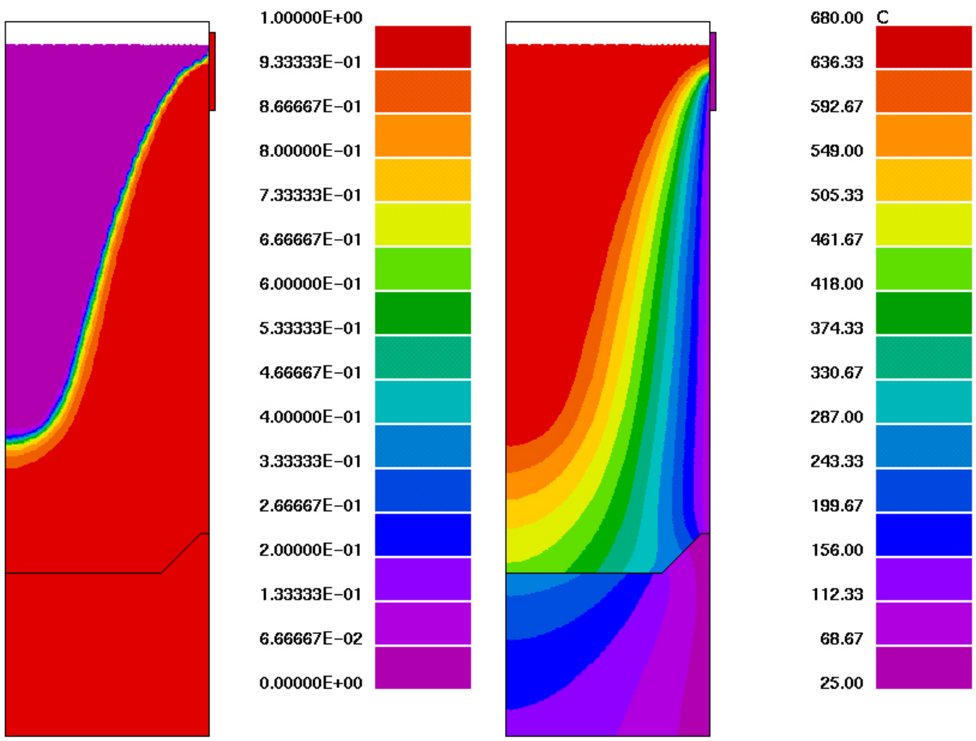

Fig 2: Solid fraction (left) and temperature (right) after nucleate boiling starts.

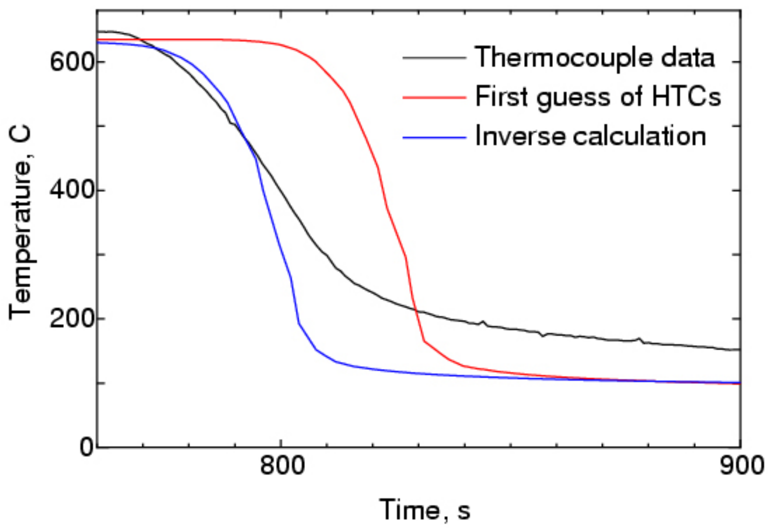

Fig 3: Temperature profiles.

2. Ingot Microstructure

Objective:

- Characterize the solidification microstructure of the DC casting ingot
- Characterize the ingot distortion

Year 2 Activities:

- The microstructure in a transverse section near the location of the surface cracking has been characterized,
- Microstructural length scales, such as grain size and secondary dendrite arm spacing, have been measured.

Results/Summary:

3.1 Techniques for revealing grain size of the alloy.

Various etching techniques were tried and an electrolytic etching technique that reveals the grain size has been selected. The etching techniques reveal the color of a grain according to the orientation of the grain. Figure 4 shows the grain size of a specimen taken from the DC cast ingot.

3.2 Grain size and secondary dendrite arm spacing distribution in the ingot.

0.5×0.5 in. samples were cut along the transverse section of an ingot. The grain size was measured using a single circle (Hilliard) procedure (ASTM specification E112). It involves the use of a circle of known circumference. The number of grain boundary intersections per unit length of the circle was counted. The mean intercept length, which is proportional to the grain size, was measured. For measuring the secondary dendrite arm spacing, Keller's solution was used to reveal the dendrite morphology. The distance between two neighboring dendrite arms was measured and taken as the secondary dendrite arm spacing.

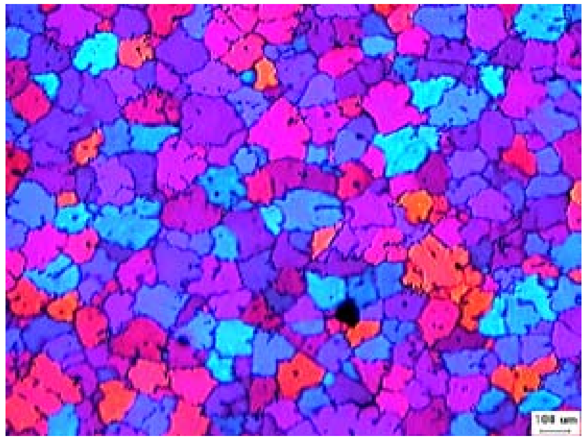

Fig 4. Grains in 3004 aluminum DC cast ingot

Figure 5 shows microstructural length scale measurements over the cross-section of a DC cast ingot. The secondary dendrite arm spacing increases with increasing distance from the surface of the ingot. This is expected since the local solidification time increases with increasing distance from the surface. The grain size results are somewhat unexpected. Large grains are observed about 9 in. from the surface. It is likely that this variation is due to the effect of fluid flow in the sump of the DC cast ingot.

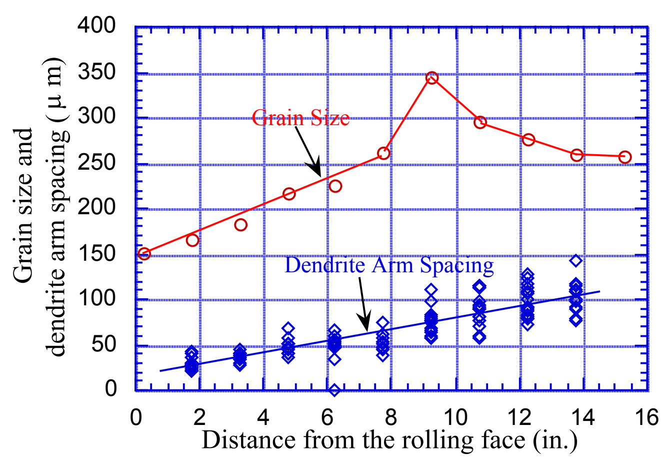

Fig 5. Microstructural length scales measured in a transverse cross section near the location where surface cracks occurred.

3.3 New features observed on microstructures at the ingot surface.

The microstructure near the ingot surface is highly non-uniform. A thin layer of fine dendrites occurs at the ingot surface. A few large dendrites coexist with small dendrites in the region adjacent to the thin layer of fine dendrites. These large dendrites likely formed earlier in the casting process and migrated to the region near the surface crack. What is surprising is that the grain size in the layer of the fine dendrites is slightly larger than the grain size further toward the center of the ingot. Thus, the region near the surface of the ingot has extremely fine small dendrites but relatively large grains. This microstructural feature has never been reported in the literature.

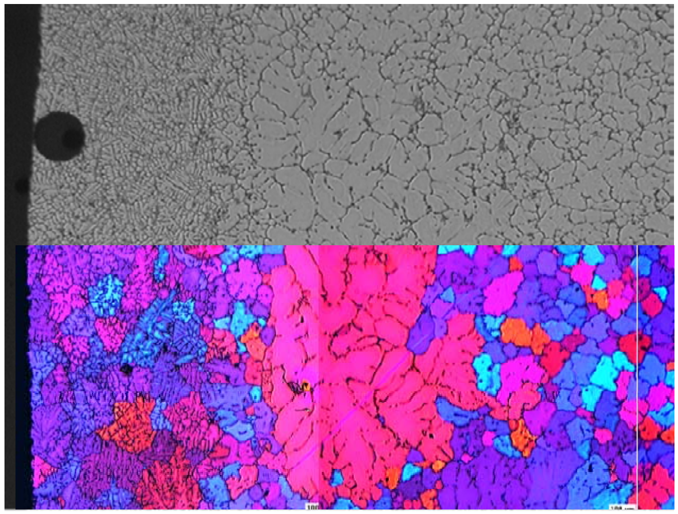

Fig 6. A thin layer near the ingot surface has been observed in which the dendrite are extremely fine but the grain sizes are somewhat larger than those further toward the center of the ingot.

3. Crack Formation and Cracking Criteria

Objective:

- To understand the mechanism of surface crack formation during D.C. Casting,
- To measure the material properties related to crack formation,
- To develop criteria for crack formation

Year 2 Activities

- Thermodynamic simulations have been carried out to determine the solidus temperature, the solid fraction curve and the segregation behavior of the alloy during solidification.
- Kinetic simulations have been carried out to determine the solidus temperature of the alloy as a function of cooling rate.
- The experimental apparatus for measuring the mechanical properties of alloys in the critical temperature range for surface cracking has been assembled.
- The apparatus is being calibrated and property measurements are ongoing.

Results/Summary

3.1.Thermodynamic simulations.

A large number of simulations have been carried for the binaries, ternaries and higher orders alloy systems that comprise a 3004 alloy. The simulations show that the solidus temperature of a 3004 alloy can be as low as 450°C, the solidus temperature of aluminum-magnesium alloys. Compared to a solidus temperature of 624°C reported in the literature for a 3004 alloy, the non-equilibrium temperature is about 174°C lower. This accounts for the fact that in the literature, surface cracking was considered to be a form of cold crack. The non-equilibrium solidus temperature is also an important parameter for experiments that determine the strength and ductility of the alloy at mushy zone temperatures.

3.2. Kinetic simulations

Another important parameter determining the mechanical properties of the alloy in the mushy zone is the variation of the non-equilibrium solidus temperature with cooling rate. The non-equilibrium temperature increases with increasing solidification time or holding time (during mechanical property tests) due to solute diffusion. If the cooling rate cannot be controlled during experimental measurements, it could result in the measurement of the properties of the solid rather than that of the semi-solid. This phenomenon is particularly important since hot tearing occurs at a very small liquid fraction, and the small amount of liquid can change rapidly due to back diffusion at mushy zone temperatures. The solidus temperature as a function of cooling rates is illustrated in Figure 7. The solidus temperature increases with decreasing cooling rate. Simulations on the dependence of the solidus temperature on the holding time during mushy zone mechanical property tests are underway.

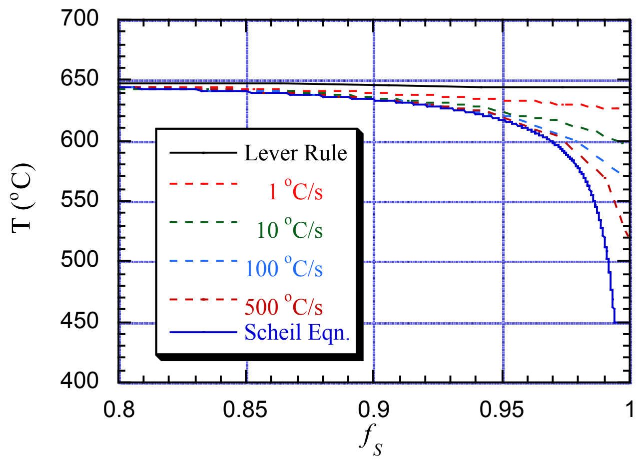

Fig 7. The solid fraction verse temperature curves for 3004 alloys at various cooling rates. The solidus temperatures are the temperatures at f_S=1.

3.3. Mushy Zone Mechanical Property Measurements

Based on a novel method proposed in Year 1 for the measurement of mechanical properties at semi-solid temperatures, the experimental apparatus has been designed and built. Simulations on heat transfer between a heating source and the specimen have been carried out. The temperature gradient in the specimen has been calculated. Based on the model predictions, an infrared furnace has been built. Specimen geometry has been determined and specimens have been machined. The locations of specimens in the ingot have been determined based on grain size measurements. The temperature distribution within a specimen during heating was measured. Six thermocouples were welded in various locations on a specimen and the temperature readings were recorded. Initial calibration of the apparatus has been carried out, and final calibration of the experimental apparatus is underway.

Figure 8 shows infrared furnace installed in the tensile test machine. Figure 9 shows a sample instrumented with thermocouples for sample and furnace calibration. Figure 10 shows the temperature profile along the gauge length of a specimen.

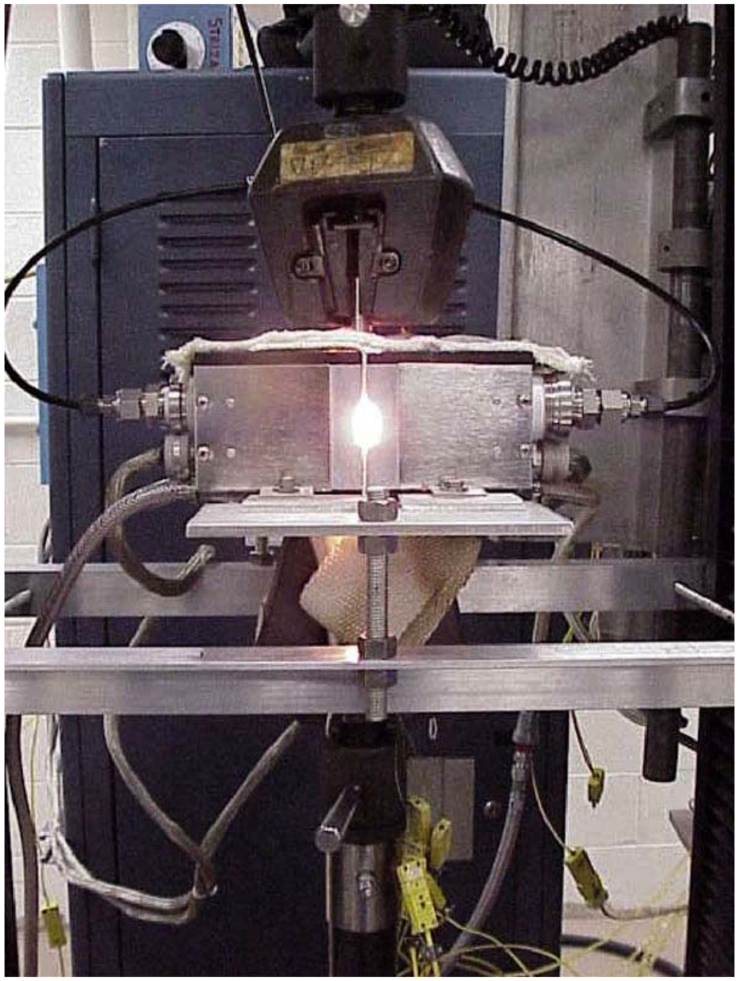

Fig 8. Setup of infrared furnace in tensile testing machine

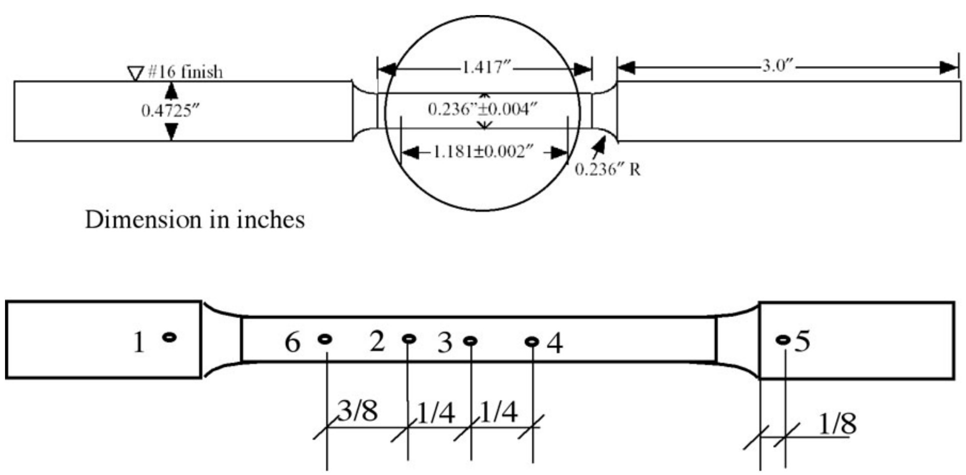

Fig. 9 Schematic Illustration of sample and thermocouple locations.

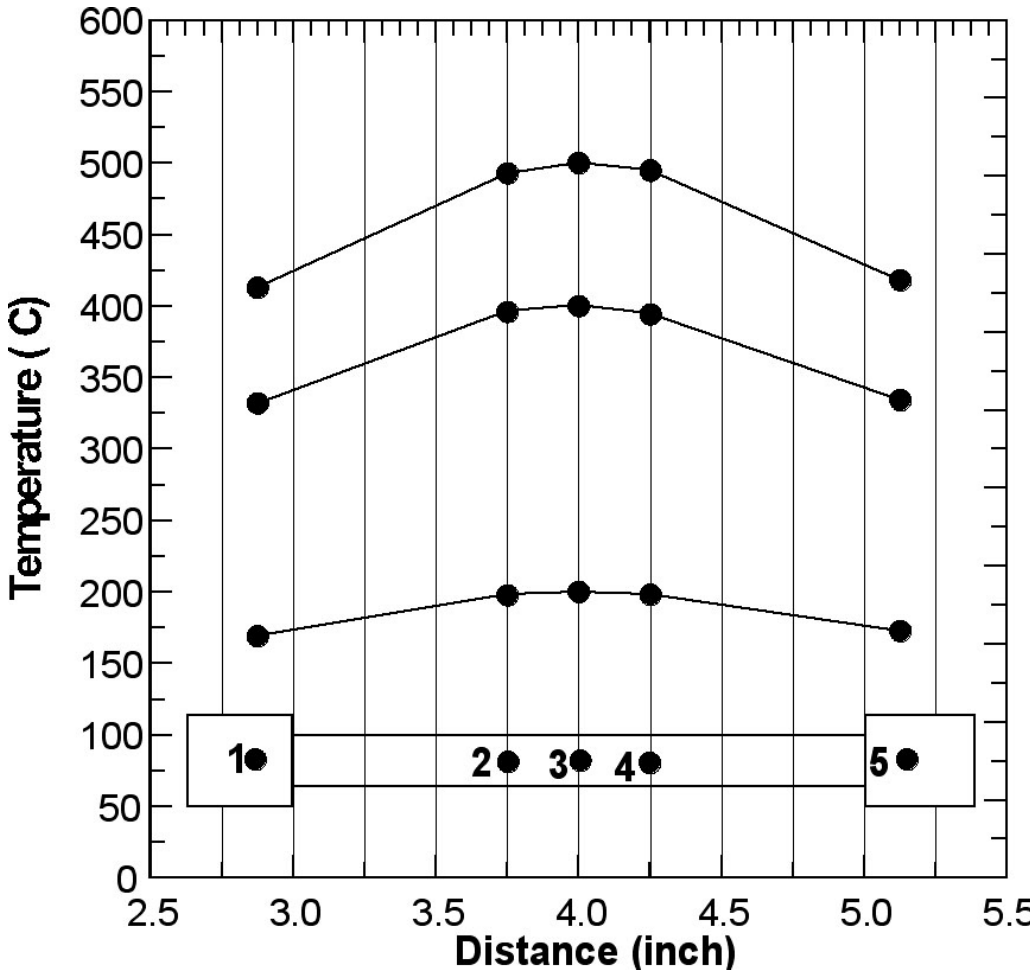

Fig 10. Temperature along specimen gauge length

Plans for the next year

Activities on all four tasks are proceeding as scheduled.

- New data acquisition software was purchased that may enhance the graphic and reporting capabilities of the system. Also, better isolation of thermocouples is planned to avoid extraneous voltage interference.
- A 2D model has been developed in ProCAST to calculate heat transfer coefficients using an inverse heat transfer technique.
- A technique has been developed to reveal the grain size of the ingot. Grains with various orientations are colored with varying colors. This makes grain size measurement possible. New microstructural features that have not been reported in the literature have been observed.
- A 3D model for stress analysis has been developed in ABAQUS. Data structures for handling the contact area between the ingot and mold, which changes in time, are automatically generated. Constitutive equations for creep have been implemented. Preliminary stress analysis and heat transfer computations have been carried out.

- Progress has been made on the measurement of high temperature material properties as follows:
    - The composition of the cracked ingot was measured.
    - A series of thermodynamic simulations have been conducted and the equilibrium and non-equilibrium solidus temperatures have been evaluated.
    - The experimental setup has been modified for better temperature control. Temperature distribution in a test specimen has been measured using 6 thermocouples.

Patents: Nil

Publications/Presentations: Nil